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Short recurrences for computing extended Krylov bases for Hermitian and unitary matrices

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Abstract It is well known that the projection of a matrix A onto a Krylov subspace span $\left\{\mathbf{h}, A\mathbf{h}, A^2\mathbf{h}, \ldots, A^{k-1}\mathbf{h}\right\}$, with $A \in \mathbb{C}^{n\times n}$ and $\mathbf{h} \in \mathbb{C}^n$, results in a Hessenberg matrix. We show that the projection of the matrix A onto an extended Krylov subspace, which is of the form span $\left\{A^{-k_r}\mathbf{h}, \ldots, A^{-2}\mathbf{h}, A^{-1}\mathbf{h}, \mathbf{h}, A\mathbf{h}, A^2\mathbf{h}, \ldots, A^{k_\ell}\mathbf{h}\right\}$, is a matrix of so-called extended Hessenberg form which can be characterized uniquely by its QR-factorization. This QR-factorization will be presented by means of a pattern of 2×2 unitary rotations. We will show how this rotation pattern leads to new insights and allows to elegantly predict the structure of the matrix. In case A is Hermitian or unitary, this extended Hessenberg matrix is banded and structured, allowing the design of short recurrence relations. For the unitary case, coupled two term recurrence relations are derived of which the coefficients capture all information necessary for a sparse factorization of the corresponding extended Hessenberg matrix.

Mathematics Subject Classification 15A23 · 65F15 · 65F25

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1 Introduction

An extended Krylov subspace is spanned by successive vectors starting from $\mathbf{h}$, taken out of the bilateral sequence

$$\ldots, A^3\mathbf{h}, A^2\mathbf{h}, A\mathbf{h}, \mathbf{h}, A^{-1}\mathbf{h}, A^{-2}\mathbf{h}, A^{-3}\mathbf{h}, \ldots, \tag{1}$$

with $A \in \mathbb{C}^{n\times n}$ and $\mathbf{v} \in \mathbb{C}^n$. The main incentive of this article is to provide theoretical foundations which can be used to efficiently compute orthonormal bases of extended Krylov subspaces. The matrix H satisfying $AQ = QH$, with Q a unitary matrix containing the orthonormal basis vectors as its columns, is a structured matrix, which will be refered to as an extended Hessenberg matrix, and which we also aim to compute in an efficient way.

Extended Krylov subspaces are fundamental tools in numerous applications including matrix functions [4,8], model order reduction [1] and Lyapunov equations [9,11], among others. For example, in [7] short recurrences for extended Krylov subspaces are investigated, relating them to Laurent polynomials, in order to evaluate expressions of the form $f(A)\mathbf{v}$ with A a large symmetric matrix and $\mathbf{v}$ a column vector.

The article is organized as follows. In Sect. 2 extended Hessenberg matrices are characterized by means of their QR-factorization, with Q factored in rotations, where the pattern of rotations exhibits a zigzag shape [2,12,14]. In Sect. 3 we establish that the matrix H satisfying $AQ = QH$, with Q a unitary matrix, is an extended Hessenberg matrix. The remainder of the paper focuses on Hermitian and unitary matrices as they exhibit a special structure giving rise to short recurrences. In Sect. 3 we show that the matrix framework built in Sect. 2 easily allows us to predict the banded structure of Hermitian and unitary extended Hessenberg matrices. This generalizes part of the theoretical results for Hermitian matrices established in [7]. Section 4 comprises a new algorithm for computing an orthonormal basis for an arbitrary extended Krylov subspace of a unitary matrix. Given the order in which the vectors are chosen from the bilateral sequence (1), the algorithm returns an orthonormal basis for the corresponding extended Krylov subspace together with a sparse factorization of the associated extended Hessenberg matrix H. The latter captures the coefficients of the recurrence relations between the orthonormal basis vectors. The orthonormal basis is retrieved recursively making use of coupled two term recurrences. The same approach of coupled two term recurrences was used in [15] to obtain the so-called CMV-shape, the latter being a specific extended Hessenberg matrix corresponding to the extended Krylov space consisting of an alternating sequence of positive and negative powers of the matrix A. In this article we provide a generalization of this approach applicable to any extended Krylov subspace.

The following notation is used throughout the article. Matrices are denoted by upper case letters $A = (a_{ij})$, the element in the matrix A on the intersection of the ith row and jth column is given by a_{ij}, and with I the identity matrix is signaled. Vectors are written in bold face and lower case letters, e.g., $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$. With $\operatorname{span}\{\mathbf{x}, \mathbf{y}, \mathbf{z}\}$ the subspace generated by vectors $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$ is meant. The standard inner product is denoted as $\langle \mathbf{x}, \mathbf{y}\rangle = \mathbf{y}^*\mathbf{x}$, with $\cdot^*$ the Hermitian conjugate. Throughout the article, Matlab's indexing is used to indicate the location of submatrices. An identity matrix with a 2×2 unitary matrix of the form

$$\begin{bmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{bmatrix}, \quad |\alpha|^2 + |\beta|^2 = 1,$$

embedded on the diagonal, will be refered to as a *rotation*. In graphical representations, a rotation matrix will be visualized by a bracket, with arrowheads targeting the rows affected by the rotation. We will only consider rotations acting on two successive rows. The order in which multiplication between brackets is carried out is just the order in which matrix multiplication is carried out if each bracket would be replaced by the matrix it represents. As an example, consider the following picture. One observes how applying the rotations affects the upper triangular matrix and generates fill-in on the first subdiagonal.

$$\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \end{bmatrix} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ & \times & \times \end{bmatrix}.$$

2 Extended Hessenberg matrices

It is well known that the projection of a matrix onto a Krylov subspace is a Hessenberg matrix. A Hessenberg matrix has a QR-factorization of the form $Q_1 Q_2 \ldots Q_{n-1} R$ where each Q_i is a rotation affecting the ith and $(i+1)$th row, resulting in a visually *descending* pattern of rotations as depicted in Fig. 1a. A matrix exhibiting a QR-factorization of the form $Q_{n-1} \ldots Q_2 Q_1 R$, where each Q_i is a rotation affecting the ith and $(i+1)$th row, will be refered to as a matrix of *inverse Hessenberg form*. In case the matrix is nonsingular, it is the inverse of a Hessenberg matrix, justifying this choice of terminology. Hence, the QR-factorization of a matrix of inverse Hessenberg form has a visually *ascending* pattern of rotations as depicted in Fig. 1b.

It will be shown in Sect. 3 that the projection of a matrix onto an extended Krylov subspace results in an *extended Hessenberg matrix*.[1] The QR-factorizations of these matrices are comprised of $n-1$ rotations and an upper triangular matrix, the positioning of the individual rotations characterizing the matrix. No specific ordering on the rotations is imposed. An extended Hessenberg matrix has a QR-factorization of the form $Q_{p_1} \ldots Q_{p_{n-1}} R$ with $p_1, \ldots, p_{n-1}$ a permutation of $1, \ldots, n-1$.

In non-factored format, extended Hessenberg matrices look like the ones in Fig. 2, possessing diagonal blocks of either Hessenberg or inverse Hessenberg form. The exact formulation is given in Definition 1.

Definition 1 A matrix H is an extended Hessenberg matrix if there exists an ordered list of indices $i_1 = 1 < i_2 < i_3 < \cdots < i_{m-1} < i_m = n$, with n the dimension of H, such that the sequence of blocks

[1] These matrices were termed *compressed matrices* in [14], as they admit an equally expensive QR-factorization as a Hessenberg matrix.

(a) Hessenberg matrix **(b)** matrix of inverse Hessenberg form

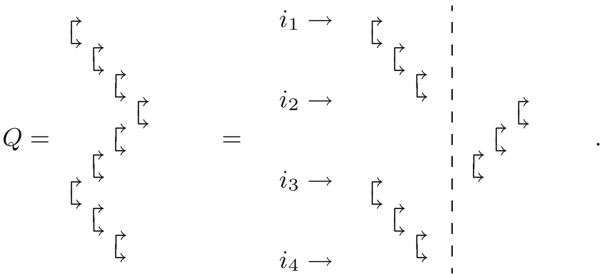
Fig. 1 Graphical depiction of two detailed QR-factorizations

$$H(i_j : i_{j+1} + \delta_j, i_j : i_{j+1} + \delta_j), \qquad \delta_j = \begin{cases} 1 & \text{if } 1 \le j < m-1, \\ 0 & \text{if } j = m-1, \end{cases}$$

are alternatingly Hessenberg and inverse Hessenberg. Also, for all $1 \le j \le m-1$, $H(r, s) = 0$, if $r > i_{j+1} + \delta_j$ and $i_j \le s < i_{j+1}$.

When discussing extended Hessenberg matrices, we will often refer to it as a block structured matrix, as these matrices are characterized by an alternating Hessenberg-inverse Hessenberg sequence of blocks on the diagonal, each block sharing a 2×2 submatrix with the next block. Note that an extended Hessenberg matrix is not a block matrix in the classical sense, as the blocks are overlapping. Therefore, standard rules involving block matrices do not apply here. However, for the ease of terminology we like to refer to the individual Hessenberg and inverse Hessenberg submatrices on the diagonal as "blocks".

Often it is more easy and insightful to work with the QR-factorization than with Definition 1. Therefore, we will examine the structure of this QR-factorization more closely. The ensemble of rotations $Q_{p_1} \dots Q_{p_{n-1}}$ can be decomposed as a product VW^H with both V and W unitary Hessenberg matrices. Roughly one can state that the matrix V encompasses the rotations associated to the Hessenberg blocks in H (descending ordering) and W the rotations linked to inverse Hessenberg blocks (ascending ordering). This *double Hessenberg* factorization was presented in a more general context in [12] and (2) displays such a factorization for a particular twisted shape. The indices i_j as stated in Definition 1 are also displayed; pointing to the beginning of each individual Hessenberg or inverse Hessenberg block. On the left of the dashed line a unitary Hessenberg matrix composed of diagonal unitary Hessenberg blocks is observed, on the right a unitary inverse Hessenberg with non compatible block diagonal structure is shown.



(2)

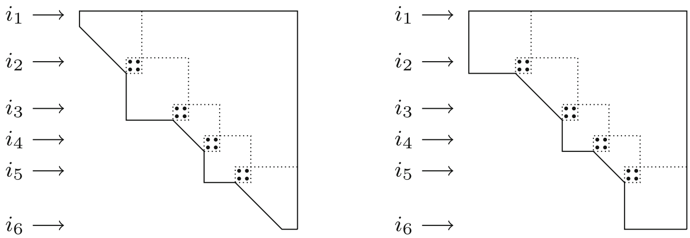


Fig. 2 Structure of an extended Hessenberg matrix and its inverse

Without loss of generality and for the ease of explanation we assume in the remainder of the text the upper left diagonal block to be Hessenberg. Then we have that the blocks $H(i_j : i_{j+1} + 1, i_j : i_{j+1} + 1)$, are Hessenberg for odd j and inverse Hessenberg for even j.

Remark 1 The inverse of an extended Hessenberg matrix is again an extended Hessenberg matrix where the Hessenberg blocks are replaced by inverse Hessenberg blocks of the same size and vice versa.

In other words, given an extended Hessenberg matrix with alternatingly Hessenberg-inverse Hessenberg structured blocks, its inverse will be an extended Hessenberg matrix with alternatingly inverse Hessenberg-Hessenberg structured blocks. Inverting the double Hessenberg factorization and passing the rotations from right to left through the upper triangular matrix[2] proves the statement. Figure 2 illustrates the block structure of an extended Hessenberg matrix, shown in the leftmost graphic, and the inverse, shown in the rightmost graphic of Fig. 2. Special attention is required when examining the overlapping elements.

3 Extended Krylov spaces

In this section it will be proved that the projection of a matrix $A \in \mathbb{C}^{n\times n}$ results in an extended Hessenberg matrix. The main result is captured in Theorem 1. First, let us introduce some terminology to characterize an extended Krylov subspace. An extended Krylov subspace is generated by not only powers of A but also of the inverse A^{-1}. By construction, a k dimensional extended Krylov subspace is spanned by k successive vectors, starting with a vector $\mathbf{h}$, out of the bilateral sequence

$$\ldots, A^3\mathbf{h}, A^2\mathbf{h}, A\mathbf{h}, \mathbf{h}, A^{-1}\mathbf{h}, A^{-2}\mathbf{h}, A^{-3}\mathbf{h}, \ldots. \tag{3}$$

The order in which the vectors are added to the subspace is crucial and recorded in a *position* vector $\mathbf{p}$ of length $n-2$, comprised of characters ℓ and r. The ℓ indicates that

[2] Given a rotation Q and an upper triangular matrix R, the product QR can be rewritten as $\tilde{R}\tilde{Q}$, where $\tilde{R}$ is upper triangular. Hence the rotation has been passed from the left to the right of the upper triangular matrix (of course rotations can also be passed from the right to the left). This shows that one can pass an entire twisted shape of rotations through an upper triangular matrix without changing the shape.

the next vector in the subspace is taken on the left, the r points out that the next vector is taken on the right of (3), e.g., the CMV-shape corresponds to the position vector $\mathbf{p} = [\ell, r, \ell, r, \ell, r, \ldots]$. By positioning positive powers of A in the bilateral sequence on the left, and inverse powers on the right we are consistent with [12,14].

Suppose that in the first $k-1$ components of $\mathbf{p}$ the symbol ℓ appears k_ℓ times and r appears k_r times ($k_r + k_\ell = k-1$), then

$$\mathcal{K}_{\mathbf{p},k}(A,\mathbf{h}) = \operatorname{span}\left\{A^{-k_r}\mathbf{h}, \ldots, A^{-2}\mathbf{h}, A^{-1}\mathbf{h}, \mathbf{h}, A\mathbf{h}, A^2\mathbf{h}, \ldots, A^{k_\ell}\mathbf{h}\right\}, \tag{4}$$

depicts the extended Krylov space of dimension $k = k_r + k_\ell + 1$. Clearly

$$\mathcal{K}_{\mathbf{p},k}(A,\mathbf{h}) = \operatorname{span}\left\{A^{-k_r}\mathbf{h}, \ldots, A^{k_\ell}\mathbf{h}\right\} = A^{-k_r}\mathcal{K}_k(A,\mathbf{h}) = A^{k_\ell}\mathcal{K}_k(A^{-1},\mathbf{h}).$$

The vectors $\mathbf{q}_1, \mathbf{q}_2, \ldots \mathbf{q}_n$ constitute an orthonormal basis of the extended Krylov subspace of the same length, hence they are the theoretical equivalent of successive orthonormalization of the vectors $A^i\mathbf{h}$ of the extended Krylov subspace. The following table presents in a comprehensible way the essential relations. Assume for now $p_1 = \ell$. The first and second row shows the position vector, the third row the vector to be orthonormalized, and the trailing row depicts the computed orthogonal vectors, which are united as the columns of a unitary matrix Q.

$\mathbf{p}$		p_1	p_2		p_{i_2-1}	p_{i_2}		p_{i_3-1}	p_{i_3}	
p_i		ℓ	ℓ	$\ldots$	ℓ	r	$\ldots$	r	ℓ	$\ldots$
vectors $\mathcal{K}_{\mathbf{p},k}(A,\mathbf{h})$	$\mathbf{h}$	$A\mathbf{h}$	$A^2\mathbf{h}$		$A^{i_2-1}\mathbf{h}$	$A^{-1}\mathbf{h}$		$A^{i_2-i_3}\mathbf{h}$	$A^{i_2}\mathbf{h}$	
columns of Q	$\mathbf{q}_1$	$\mathbf{q}_2$	$\mathbf{q}_3$		$\mathbf{q}_{i_2}$	$\mathbf{q}_{i_2+1}$		$\mathbf{q}_{i_3}$	$\mathbf{q}_{i_3+1}$	

$\mathbf{p}$		p_{i_4-1}	p_{i_4}		p_{i_5-1}	p_{i_5}	
p_i	$\ldots$	ℓ	r	$\ldots$	r	ℓ	$\ldots$
vectors $\mathcal{K}_{\mathbf{p},k}(A,\mathbf{h})$		$A^{i_2-i_3+i_4-1}\mathbf{h}$	$A^{i_2-i_3-1}\mathbf{h}$		$A^{i_2-i_3-i_4+i_5+1}\mathbf{h}$	$A^{i_2-i_3+i_4}\mathbf{h}$	
columns of Q		$\mathbf{q}_{i_4}$	$\mathbf{q}_{i_4+1}$		$\mathbf{q}_{i_5}$	$\mathbf{q}_{i_5+1}$	

A non-interrupted sequence of vectors out of the two trailing rows starting with $\mathbf{h}$ and $\mathbf{q}_1$ generate, by construction, identical subspaces:

$$\operatorname{span}\left\{A^{-k_r}\mathbf{h}, \ldots, A^{k_\ell}\mathbf{h}\right\} = \operatorname{span}\{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_k\}.$$

The inclusion $A\mathcal{K}_k(A,\mathbf{h}) \subset \mathcal{K}_{k+1}(A,\mathbf{h})$ for standard Krylov subspaces is a key item in the derivation of the Hessenberg structure capturing the recurrence coefficients for the orthogonal vectors. For the extended case, the values of the position vector affect the relations.

Lemma 1 (Lemma 3.6 in [14]) *For $k = 1, \ldots, n-2$,*

(a) *if $p_k = \ell$, then $A\mathcal{K}_{\mathbf{p},k}(A,\mathbf{h}) \subseteq \mathcal{K}_{\mathbf{p},k+1}(A,\mathbf{h})$.*
(b) *if $p_k = r$, then $A^{-1}\mathcal{K}_{\mathbf{p},k}(A,\mathbf{h}) \subseteq \mathcal{K}_{\mathbf{p},k+1}(A,\mathbf{h})$.*

Once the position vector is set, we are interested in the matrix H satisfying $AQ = QH$, Q unitary. In [12,14] the structure of the matrix H was already established for the generic matrix case. In the spirit of this article, we will, however, deduce an alternative proof along the same lines as for the Hessenberg setting. The matrix H will be an extended Hessenberg matrix, which has Hessenberg and inverse Hessenberg blocks on its diagonal. More precisely, based on a given position vector $\mathbf{p}$ we define the characterizing indices i_j as follows: $i_1 = 1$ and i_j is the position k such that the $(j-1)$th transition from ℓ to r, or r to ℓ takes place between p_{k-1} and p_k. The list is closed by a trailing $i_j = n$, where n is the dimension of A. We will prove now that the matrix H meets the extended Hessenberg matrix constraints (reconsider Definition 1 in relation with the indices i_j). To do so, we rely on the following result:

Lemma 2 (Corollary of the Nullity Theorem [13]) *Suppose $A \in \mathbb{R}^{n\times n}$ is a nonsingular matrix, and α, β are nonempty subsets of N with $|\alpha| < n$ and $|\beta| < n$, N being the index set $\{1, 2, \ldots, n\}$ and $|\cdot|$ denoting the cardinality of a set. Then*

$$\mathit{rank}\left(A^{-1}(\alpha;\beta)\right) = \mathit{rank}\,(A(N\backslash\beta; N\backslash\alpha)) + |\alpha| + |\beta| - n.$$

Theorem 1 *Given a matrix $A \in \mathbb{C}^{n\times n}$ and a vector $\mathbf{h} \in \mathbb{C}^n$. Assuming no breakdown, then the projection of A onto the extended Krylov space $\mathcal{K}_{\mathbf{p},n}(A, \mathbf{h})$ results in an extended Hessenberg matrix.*

Proof Reconsidering the relation $AQ = QH$ of which we want to extract the structure of H, we see that for $i_1 = 1 \leq i \leq i_2 - 1$, $A\mathbf{q}_i$ is a linear combination of the vectors $\mathbf{q}_1, \ldots, \mathbf{q}_{i+1}$. This statement results also from Lemma 1: the values of $p_1, \ldots, p_{i_2-1}$ all equal ℓ and therefore for $1 \leq i \leq i_2 - 1$

$$A[\mathbf{q}_1, \ldots, \mathbf{q}_i] = [\mathbf{q}_1, \ldots \mathbf{q}_{i+1}]H(1 : i+1, 1 : i),$$

with $H(1 : i_2, 1 : i_2)$ thus a Hessenberg matrix. The conclusion on the structure can be extended to all orthogonal vectors $\mathbf{q}_i$ for which $p_i = \ell$. More precisely, Lemma 1 implies the general relations

$$A[\mathbf{q}_1, \ldots, \mathbf{q}_i] = [\mathbf{q}_1, \ldots, \mathbf{q}_{i+1}]H(1 : i+1, 1 : i), \quad \text{for } i_j \leq i \leq i_{j+1} - 1,\ j \text{ odd},$$

imposing thus a Hessenberg structure on the blocks $H(i_j : i_{j+1}, i_j : i_{j+1})$ for odd j.

Unfortunately there is not much to say about the other diagonal blocks. Lemma 1 only implies that for $i_j \leq i \leq i_{j+1}$, j even, with $p_{i_{j+1}}$ thus the earliest next appearance of ℓ that

$$A\mathcal{K}_{\mathbf{p},i} \subseteq \mathcal{K}_{\mathbf{p},i_{j+1}}.$$

This yields

$$A[\mathbf{q}_1, \ldots, \mathbf{q}_i] = [\mathbf{q}_1, \ldots, \mathbf{q}_{i_{j+1}+1}]H(1 : i_{j+1} + 1, 1 : i),$$

and we get thus a dense block $H(i_j : i_{j+1} + 1, i_j : i_{j+1} + 1)$ for even j.

To prove the inverse Hessenberg structure of the dense diagonal blocks we use the inverse relation $A^{-1}Q = QH^{-1}$. First we prove that the blocks $H^{-1}(i_j : i_{j+1}, i_j : i_{j+1})$ are Hessenberg matrices, for even j. To construct the matrix Q starting with A^{-1}, the elements in the position vector need to be exchanged, i.e., symbols r become ℓ's and vice versa. In this way exactly the same orthonormal basis vectors are found leading thus to an identical matrix Q. Identical reasoning as in the previous paragraph leads us to the Hessenberg structure of the diagonal blocks under consideration. Note that this implies that the diagonal blocks $H^{-1}(i_j : i_{j+1}+1, i_j : i_{j+1}+1)$ are Hessenberg matrices. Therefore, Lemma 2 implies that

$$\begin{aligned}\operatorname{rank}\left(H(i_j+k:n, 1:i_j+l)\right) &= \operatorname{rank}\left(H^{-1}(i_j+l+1:n, 1:i_j+k-1)\right)\\ &\quad +l-k+1,\\ &\le (k-l)+(l-k+1)=1,\end{aligned}$$

with $0 \le l \le k \le i_{j+1} - i_j$, the last equality being due to the fact that $H^{-1}(i_j : i_{j+1}+1, i_j : i_{j+1}+1)$ is a Hessenberg matrix. As

$$\operatorname{rank}\left(H(i_j+k:n, 1:i_j+l)\right) \ge \operatorname{rank}\left(H(i_j+k:i_{j+1}, i_j:i_j+l)\right),$$

it follows that all submatrices of $H(i_j : i_{j+1}+1, i_j : i_{j+1}+1)$, j even, below the first superdiagonal are of rank at most one, establishing the inverse Hessenberg structure. □

3.1 Hermitian matrices

In case the matrix A is Hermitian, a generalization of the Lanczos algorithm can be constructed for computing the orthonormal basis vectors for an extended Krylov subspace. In [7] short recurrence relations are derived for the position vectors $\mathbf{p} = [\ell, r, \ell, r, \ell, \ldots]$ and $\mathbf{p} = [\ell, \ell, r, \ell, \ell, r, \ldots]$. Also the corresponding extended Hessenberg matrix H, i.e., such that $AQ = QH$ with Q unitary, shows to have a banded structure. The results are established by making use of orthogonal Laurent polynomials.

In this section we propose a different approach and combine Theorem 1, which predicts the structure of the matrix H as a function of the position vector $\mathbf{p}$ and the relation $H = H^*$, in order to derive the banded structure of the matrix H. It follows that any Hermitian extended Hessenberg matrix H has a banded structure, the bandwidth depending on the structure of the position vector $\mathbf{p}$. Position vectors containing long strings of consecutive r's result in matrices with larger bandwidth, i.e., the larger the difference $i_{j+1} - i_j$ (with j even if the first element of $\mathbf{p}$ is an ℓ), the larger the bandwidth. This can also be seen in Fig. 2, where a succession of r's corresponds to an inverse Hessenberg block on the diagonal, whereas a succession of ℓ's corresponds to a Hessenberg block on the diagonal. Depending on the bandwidth, recurrences of limited length are obtained. These recurrences, together with Algorithm 1 below are

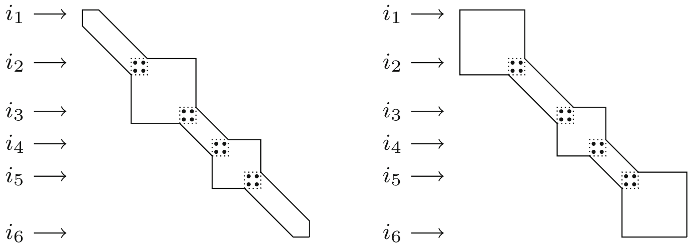


Fig. 3 Structure of an Hermitian extended Hessenberg matrix and its inverse

applicable to any configuration of the position vector $\mathbf{p}$, hence they can be seen as a generalization of the recurrence relations derived in [7].

Figure 2 shows the structure of a general extended Hessenberg matrix together with its inverse. Projecting the Hermitian conjugate of both matrices on themselves, the zero structure as depicted in Fig. 3 is found. It is assumed that the position vector $\mathbf{p}$ starts with the symbol ℓ.

The values of $p_{i_j}, p_{i_j+1}, \ldots, p_{i_{j+1}-1}$, for j odd, all equal ℓ. Hence Lemma 1(a) and the relation $H^* = H$ imply the recurrence relations

$$\beta \mathbf{v}_{i+1} = A\mathbf{v}_i - \sum_{k=i-1}^{i} \alpha_k \mathbf{q}_k, \qquad i_j + 2 \le i \le i_{j+1} - 1, \tag{5}$$

with $\alpha_k = \mathbf{v}_k^T A\mathbf{v}_i$, $\beta = \sqrt{||A\mathbf{v}_i||_2 - \sum_{k=i-1}^{i} |\alpha_k|^2}$,

$$\gamma \mathbf{v}_{i_j+1} = A\mathbf{v}_{i_j} - \sum_{k=i_{j-1}}^{i_j} \delta_k \mathbf{v}_k, \tag{6}$$

with $\delta_k = \mathbf{v}_k^T A\mathbf{v}_{i_j}$, $\gamma = \sqrt{||A\mathbf{v}_{i_j}||_2 - \sum_{k=i_{j-1}}^{i_j} |\delta_k|^2}$, and

$$\varepsilon \mathbf{v}_{i_j+2} = A\mathbf{v}_{i_j+1} - \sum_{k=i_{j-1}}^{i_j+1} \chi_k \mathbf{q}_k, \tag{7}$$

with $\chi_k = \mathbf{v}_k^T A\mathbf{v}_{i_j+1}$, $\varepsilon = \sqrt{||A\mathbf{v}_{i_j+1}||_2 - \sum_{k=i_{j-1}}^{i_j+1} |\chi_k|^2}$.

The values of $p_{i_j}, p_{i_j+1}, \cdots, p_{i_{j+1}-1}$, for j even, all equal r. Hence, by making use of Lemma 1(b) and $\left(H^{-1}\right)^* = H^{-1}$ the same formulas for odd j hold with A replaced by A^{-1}. We obtain

$$\beta \mathbf{v}_{i+1} = A^{-1}\mathbf{v}_i - \sum_{k=i-1}^{i} \alpha_k \mathbf{v}_k, \qquad i_j + 2 \le i \le i_{j+1} - 1, \tag{8}$$

with $\alpha_k = \mathbf{v}_k^T A^{-1}\mathbf{v}_i$, $\beta = \sqrt{||A^{-1}\mathbf{v}_i||_2 - \sum_{k=i-1}^{i} |\alpha_k|^2}$,

$$\gamma \mathbf{v}_{i_j+1} = A^{-1}\mathbf{v}_{i_j} - \sum_{k=i_{j-1}}^{i_j} \delta_k \mathbf{v}_k, \tag{9}$$

with $\delta_k = \mathbf{v}_k^T A^{-1}\mathbf{v}_{i_j}$, $\gamma = \sqrt{||A^{-1}\mathbf{v}_{i_j}||_2 - \sum_{k=i_{j-1}}^{i_j} |\delta_k|^2}$, and

$$\varepsilon \mathbf{v}_{i_j+2} = A^{-1}\mathbf{v}_{i_j+1} - \sum_{k=i_{j-1}}^{i_j+1} \chi_k \mathbf{v}_k, \tag{10}$$

with $\chi_k = \mathbf{v}_k^T A^{-1}\mathbf{v}_{i_j+1}$, $\varepsilon = \sqrt{||A^{-1}\mathbf{v}_{i_j+1}||_2 - \sum_{k=i_{j-1}}^{i_j+1} |\chi_k|^2}$.

If the value of the first entry of the position vector $\mathbf{p}$ is r, the same recurrence relations hold with A and A^{-1} swapped. The above recurrence relations are implemented in Algorithm 1. Furthermore, in [7] various numerical experiments show these type of recurrence relations often lead to more accurate results than the standard Lanczos algorithm in the approximation of expressions of the form $f(A)\mathbf{v}$. For several functions, such as $\exp(-x)/x$, $\sqrt{x}$, $\exp(-\sqrt{x})$, ... it is established that projecting the matrix onto an extended Krylov subspace and exploiting the fact that the resulting extended Hessenberg matrix is banded, gives rise to better results than using the standard Lanczos algorithm. As Algorithm 1 is applicable to any position vector $\mathbf{p}$, the algorithm has the potential to become adaptive and give the user the opportunity to adjust the position vector at runtime in order to improve convergence. However, the question of how to choose an optimal position vector is a difficult one and beyond the scope of this article.

We will now apply the above results to the examples discussed in [7] and show how for these specific cases the recurrences above reduce to the ones stated in [7]. In the remainder of this section we switch to the index notation used in [7], i.e., the index m denotes that the corresponding vector is the result of orthonormalizing $A^m\mathbf{h}$ with $\mathbf{h}$ the starting vector against the previously computed orthonormal vectors. For the first example consider the position vector $\mathbf{p} = [\ell, r, \ell, r, \ell, \ldots]$. We aim to compute the corresponding orthonormal basis $\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_{-1}, \mathbf{v}_2, \mathbf{v}_{-2}, \ldots$. As in this case the indices $i_1, i_2, \ldots, i_n$ are consecutive numbers, Eqs. (5), (7), (8) and (10) do not apply. Hence, the resulting basis is computed by alternatingly applying Eqs. (6) and (9) which, using the notation of [7], transform into the recurrence relations

$$\begin{aligned}
\delta_{m+1}\mathbf{v}_{m+1} &= (A - \alpha_{-m} I_n)\mathbf{v}_{-m} - \alpha_m \mathbf{v}_m, \quad \alpha_j = \mathbf{v}_j^T A \mathbf{v}_{-m},\\
\delta_{-m}\mathbf{v}_{-m} &= (A^{-1} - \beta_m I_n)\mathbf{v}_m - \beta_{-m+1}\mathbf{v}_{-m+1}, \quad \beta_j = \mathbf{v}_j^T A^{-1}\mathbf{v}_m,
\end{aligned}$$

δ_{m+1}, δ_{-m} orthonormalization factors to make the corresponding vector of unit length. These are also the recurrence relations as stated in [7].

Another example which is investigated in [7] is the position vector $\mathbf{p} = [\ell, \ell, r, \ell, \ell, r, \ldots]$, giving rise to an orthonormal basis $\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_{-1}, \mathbf{v}_3, \mathbf{v}_4, \mathbf{v}_{-2}, \ldots$.

Algorithm 1 Algorithm for computing orthonormal extended Krylov bases for Hermitian matrices.

Require: Hermitian matrix $A \in \mathbb{C}^{n\times n}$, starting vector $\mathbf{h}$, position vector $\mathbf{p}$ (starting with ℓ) with $i_m = n$

$\mathbf{v}_1 = \mathbf{h}/||\mathbf{h}||$;
$\mathbf{w} = A\mathbf{v}_1$;
$\alpha_1 = \mathbf{v}_1^T\mathbf{w}$; $\mathbf{w} = \mathbf{w} - \alpha_1\mathbf{v}_1$;
$\beta = ||\mathbf{w}||$; $\mathbf{v}_2 = \mathbf{w}/\beta$;
for $i = 2 \to i_2 - 1$ **do**
  $\mathbf{w} = A\mathbf{v}_i$;
  $\alpha_{i-1} = \mathbf{v}_{i-1}^T\mathbf{w}$; $\mathbf{w} = \mathbf{w} - \alpha_{i-1}\mathbf{v}_{i-1}$;
  $\alpha_i = \mathbf{v}_i^T\mathbf{w}$; $\mathbf{w} = \mathbf{w} - \alpha_i\mathbf{v}_i$;
  $\beta = ||\mathbf{w}||$; $\mathbf{v}_{i+1} = \mathbf{w}/\beta$;
end for
for $j = 2 \to m - 1$ **do**
  if j odd **then**
    $\mathbf{w} = A\mathbf{v}_{i_j}$;
  else
    $\mathbf{w} = A^{-1}\mathbf{v}_{i_j}$;
  end if
  for $k = i_{j-1} \to i_j$ **do**
    $\delta_k = \mathbf{v}_k^T\mathbf{w}$; $\mathbf{w} = \mathbf{w} - \delta_k\mathbf{v}_k$;
  end for
  $\gamma = ||\mathbf{w}||$; $\mathbf{v}_{i_j+1} = \mathbf{w}/\gamma$;
  if j odd **then**
    $\mathbf{w} = A\mathbf{v}_{i_j+1}$;
  else
    $\mathbf{w} = A^{-1}\mathbf{v}_{i_j+1}$;
  end if
  for $k = i_{j-1} \to i_j + 1$ **do**
    $\chi_k = \mathbf{v}_k^T\mathbf{w}$; $\mathbf{w} = \mathbf{w} - \chi_k\mathbf{v}_k$;
  end for
  $\varepsilon = ||\mathbf{w}||$; $\mathbf{v}_{i_j+1} = \mathbf{w}/\varepsilon$;
  for $i = i_j + 2 \to i_{j+1} - 1$ **do**
    if j odd **then**
      $\mathbf{w} = A\mathbf{v}_i$;
    else
      $\mathbf{w} = A^{-1}\mathbf{v}_i$
    end if
    $\alpha_{i-1} = \mathbf{v}_{i-1}^T\mathbf{w}$; $\mathbf{w} = \mathbf{w} - \alpha_{i-1}\mathbf{v}_{i-1}$;
    $\alpha_i = \mathbf{v}_i^T\mathbf{w}$; $\mathbf{w} = \mathbf{w} - \alpha_i\mathbf{v}_i$;
    $\beta = ||\mathbf{w}||$; $\mathbf{v}_{i+1} = \mathbf{w}/\beta$;
  end for
end for
  return $(\mathbf{v}_i)$

Examining the position vector $\mathbf{p}$, one concludes that the corresponding basis can be computed by alternatingly applying Eqs. (6), (7) and (9). Again, using the notation of [7], these equations transform into the recurrence relations

$$
\begin{aligned}
\delta_{2m+1}\mathbf{v}_{2m+1} &= (A-\alpha_{-m,-m}I_n)\mathbf{v}_{-m} - \alpha_{-m,2m}\mathbf{v}_{2m},\\
\delta_{2m}\mathbf{v}_{2m} &= (A-\alpha_{2m-1,2m-1}I_n)\mathbf{v}_{2m-1} - \alpha_{2m-1,-m+1}\mathbf{v}_{-m+1}\\
&\quad -\alpha_{2m-1,2m-2}\mathbf{v}_{2m-2},\\
\delta_{-m}\mathbf{v}_{-m} &= (A^{-1}-\beta_{2m,2m}I_n)\mathbf{v}_{2m} - \beta_{2m,-m+1}\mathbf{v}_{-m+1} - \beta_{2m,2m-1}\mathbf{v}_{2m-1},
\end{aligned}
$$

with $\alpha_{j,k} = \mathbf{v}_j^T A\mathbf{v}_k$, $\beta_{j,k} = \mathbf{v}_j^T A^{-1}\mathbf{v}_k$, and δ_j a positive factor making the corresponding vector of unit length. Again, these are also the recurrence relations as stated in [7].

3.2 Unitary matrices

The class of unitary matrices in this extended Krylov space setting exhibits the most intriguing properties, as recently much attention is paid to the rediscovery of the so-called CMV-matrix [3,10,15]. The pentadiagonal unitary matrix associated to an alternating appearance of ℓ and r in the position vector is a CMV-matrix. Generalizations for other types of position vectors can, e.g., be found in [2].

The alternating appearance of ℓ's and r's implies $i_j = j$. The leftmost graphic in Fig. 4 shows the resulting pentadiagonal structure capturing the recurrence coefficients. The nonzero matrix elements are represented by bullets. We will prove now in a different way that this structure is correct.

The second graph reveals the structure of the lower triangular part in correspondence to Sect. 3. Projecting the structure of the inverse matrix on the upper Hessenberg part, using the relation $U^* = U^{-1}$, nicely provides us the zero structure of the upper triangular part of the matrix H. The elements surrounded by a dotted line belong to a Hessenberg block, the ones surrounded by a dense line make up an inverse Hessenberg matrix. The inverse is characterized by a simple interchange of inverse and Hessenberg blocks. The third graph provides the structure, with marked blocks, of the inverse.

The same reasoning applies to any type of position vector. As an example, consider the position vector $\mathbf{p} = [\ell, \ell, r, \ell, r, r, \ell, r, \ldots]$. The latter gives rise to the extended Hessenberg matrix as depicted in the leftmost graphic in Fig. 5. The rightmost graphic of Fig. 5 represents the inverse. Again the structure of the lower triangular part is retrieved in correspondence to Sect. 3, whereas the zero structure of the upper triangular part results from the relation $U^* = U^{-1}$.

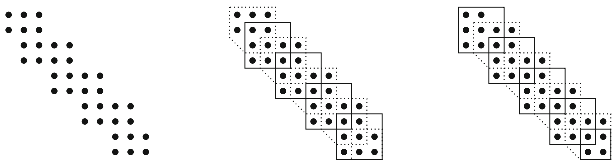


Fig. 4 CMV structure

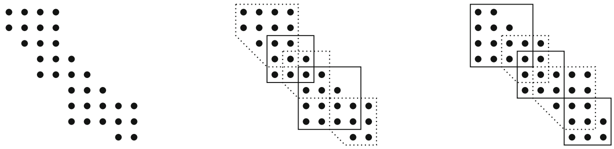


Fig. 5 Interpretations of an extended unitary Hessenberg matrix and its inverse

4 Two term recursions for unitary matrices

In this section an algorithm will be proposed for computing an orthonormal basis for an extended Krylov subspace, based on coupled two term recurrences, i.e., vectors are computed successively by only making use of two of the previously computed vectors. In [15] it is shown that the vectors which consitute a basis for the extended Krylov subspace corresponding to the position vector $\mathbf{p} = [\ell, r, \ell, r, \ell, \ldots]$ can be computed recursively with a coupled two term recurrence. The term 'coupled' refers to the fact that the latter basis is computed simultaneously with a basis for the extended Krylov subspace corresponding to the position vector $\mathbf{p} = [r, \ell, r, \ell, \ldots]$. Projecting the unitary matrix under consideration on this extended Krylov subspace, gives rise to a matrix of CMV-form. Our method places the approach used in [15] in a more general framework, resulting in an algorithm which is able to compute an extended Krylov basis for any position vector $\mathbf{p}$.

In the first subsection we revisit the CMV-shape and apply our method to derive the coupled two term recurrences as stated in [15]. The second subsection discusses the intended generalization, illustrating its applicability in an example in the third subsection. Finally, in the fourth subsection a more general example and the corresponding algorithm are provided.

4.1 CMV shape

Given a unitary matrix U and a random starting vector $\mathbf{h}$, the sequence

$$\mathbf{h}, U\mathbf{h}, U^{-1}\mathbf{h}, U^2\mathbf{h}, U^{-2}\mathbf{h}, U^3\mathbf{h}, U^{-3}\mathbf{h}, \ldots$$

corresponding to an alternating appearance of ℓ's and r's, can be orthonormalized using two term recursions. To this end, we orthonormalize this sequence simultaneously with the sequence

$$\mathbf{h},\ U^{-1}\mathbf{h},\ U\mathbf{h},\ U^{-2}\mathbf{h},\ U^2\mathbf{h},\ U^{-3}\mathbf{h},\ U^3\mathbf{h},\ \ldots.$$

We denote the orthonormal basis associated with the first sequence by $(\mathbf{v}_k)$, and that associated with the second sequence by $(\mathbf{w}_k)$. This means we will successively compute the basis vectors

$$\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_{-1}, \mathbf{v}_2, \mathbf{v}_{-2}, \mathbf{v}_3, \mathbf{v}_{-3}, \ldots,$$

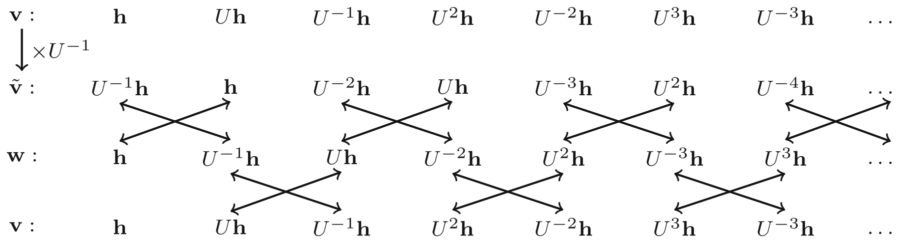


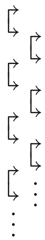
Fig. 6 Links between the sequences corresponding to the bases $(\mathbf{v}_k)$ and $(\mathbf{w}_k)$

as well as

$$\mathbf{w}_0, \mathbf{w}_{-1}, \mathbf{w}_1, \mathbf{w}_{-2}, \mathbf{w}_2, \mathbf{w}_{-3}, \mathbf{w}_3, \ldots,$$

where $\mathbf{v}_k$, $\mathbf{w}_k$ denote the result of orthonormalizing $U^k\mathbf{h}$ against all previously computed vectors of $(\mathbf{v}_k)$, $(\mathbf{w}_k)$ respectively. We will now present our method as a specific instance applied to CMV, deriving the same coupled two term recurrences as in [15].

The position vector $\mathbf{p} = [\ell, r, \ell, r, \ell, r, \ldots]$ corresponds to the sequence of rotations (11).



(11)

Consider the scheme depicted in Fig. 6, which consists of three sequences of vectors. After orthormalization these give rise to the bases $(\mathbf{v}_k)$, $(\tilde{\mathbf{v}}_k)$ and $(\mathbf{w}_k)$. The sequences are constructed as follows. The sequence corresponding to $(\tilde{\mathbf{v}}_k)$ is obtained by multiplying the sequence corresponding to $(\mathbf{v}_k)$ with the unitary factor U^{-1}. This immediately implies the relation $\mathbf{v}_k = U\tilde{\mathbf{v}}_{k-1}$ for all $k \in \mathbb{Z}$. Next consider the twisted pattern of rotations as depicted in (11). Intuitively, the locations of the rotations in the first column of this pattern link the sequences corresponding to the bases $(\tilde{\mathbf{v}}_k)$ and $(\mathbf{w}_k)$, and the locations of the rotations in the second column link the sequences corresponding to the bases $(\mathbf{w}_k)$ and $(\mathbf{v}_k)$. More precisely, the sequence corresponding to $(\mathbf{w}_k)$ can be derived from that of $(\tilde{\mathbf{v}}_k)$ by swapping neighbouring elements whenever there is a rotation acting on the same positions in the first column. Analogously, the sequence corresponding to $(\mathbf{v}_k)$ can be derived from that of $(\mathbf{w}_k)$ be swapping neighbouring elements whenever there is a rotation acting on the same positions in the second column. This is depicted by the arrows in Fig. 6.

Note that the crosses in Fig. 6 follow the same pattern as the rotations in (11), i.e., if we go the left in the pattern of rotations (11), we go down in Fig. 6; if we go the right in the pattern of rotations (11), we go up in Fig. 6.

Lemma 3 *Using the scheme of Fig. 6, the following equalities can be derived:*

$$\mathit{span}\{\tilde{\mathbf{v}}_{-1}, \ldots, \tilde{\mathbf{v}}_{-k}, \tilde{\mathbf{v}}_{k-1}\} = \mathit{span}\{\mathbf{w}_0, \ldots, \mathbf{w}_{k-1}, \mathbf{w}_{-k}\}, \tag{12}$$

$$\mathit{span}\{\tilde{\mathbf{v}}_{-1}, \ldots, \tilde{\mathbf{v}}_{-k}, \tilde{\mathbf{v}}_{k-1}\} = \mathit{span}\{\tilde{\mathbf{v}}_{-1}, \ldots, \tilde{\mathbf{v}}_{-k}, \mathbf{w}_{k-1}\}, \tag{13}$$

$$\mathit{span}\{\mathbf{w}_0, \ldots, \mathbf{w}_{k-1}, \mathbf{w}_{-k}\} = \mathit{span}\{\mathbf{w}_0, \ldots, \mathbf{w}_{k-1}, \tilde{\mathbf{v}}_{-k}\}, \tag{14}$$

and

$$\mathit{span}\{\mathbf{w}_0, \ldots, \mathbf{w}_{-k}, \mathbf{w}_k\} = \mathit{span}\{\mathbf{v}_0, \ldots, \mathbf{v}_k, \mathbf{v}_{-k}\}, \tag{15}$$

$$\mathit{span}\{\mathbf{w}_0, \ldots, \mathbf{w}_{-k}, \mathbf{w}_k\} = \mathit{span}\{\mathbf{w}_0, \ldots, \mathbf{w}_{-k}, \mathbf{v}_k\}, \tag{16}$$

$$\mathit{span}\{\mathbf{v}_0, \ldots, \mathbf{v}_k, \mathbf{v}_{-k}\} = \mathit{span}\{\mathbf{v}_0, \ldots, \mathbf{v}_k, \mathbf{w}_{-k}\}, \tag{17}$$

for all $k > 0$.

Proof We provide a proof only for equalities (12)–(14) as equalities (15)–(17) follow analogously. Equality (12) is derived from the fact that the sequences in Fig. 6 underlying the bases $(\tilde{\mathbf{v}}_k)$ and $(\mathbf{w}_k)$ are equal to each other up to permutation, and therefore span the same subspaces. More precisely, we have that

$$\begin{aligned}
\operatorname{span}\{\tilde{\mathbf{v}}_{-1}, \tilde{\mathbf{v}}_0, \ldots, \tilde{\mathbf{v}}_{-k}, \tilde{\mathbf{v}}_{k-1}\} &= \operatorname{span}\{U^{-1}\mathbf{h}, \mathbf{h}, \ldots, U^{-k}\mathbf{h}, U^{k-1}\mathbf{h}\} \\
&= \operatorname{span}\{\mathbf{h}, U^{-1}\mathbf{h}, \ldots, U^{k-1}\mathbf{h}, U^{-k}\mathbf{h}\} \\
&= \operatorname{span}\{\mathbf{w}_0, \mathbf{w}_{-1}, \ldots, \mathbf{w}_{k-1}, \mathbf{w}_{-k}\},
\end{aligned}$$

thereby establishing Eq. (12). Next note that $\mathbf{w}_{k-1}$ is contained in

$$\begin{aligned}
&\operatorname{span}\{\mathbf{h}, U^{-1}\mathbf{h}, \ldots, U^{k-2}\mathbf{h}, U^{-k+1}\mathbf{h}, U^{k-1}\mathbf{h}\} \\
&\quad = \operatorname{span}\{\mathbf{w}_0, \mathbf{w}_{-1}, \ldots, \mathbf{w}_{k-2}, \mathbf{w}_{-k+1}, U^{k-1}\mathbf{h}\} \\
&\quad = \operatorname{span}\{\tilde{\mathbf{v}}_{-1}, \tilde{\mathbf{v}}_0, \ldots, \tilde{\mathbf{v}}_{-k+1}, \tilde{\mathbf{v}}_{k-2}, U^{k-1}\mathbf{h}\},
\end{aligned}$$

where the last equality is due to (12). A key observation is that when writing $\mathbf{w}_{k-1}$ down as a linear combination of the vectors $\tilde{\mathbf{v}}_{-1}, \tilde{\mathbf{v}}_0, \ldots, \tilde{\mathbf{v}}_{-k+1}, \tilde{\mathbf{v}}_{k-2}$ and $U^{k-1}\mathbf{h}$, the coefficient in the direction of $U^{k-1}\mathbf{h}$ is nonzero.

Hence, we obtain

$$\begin{aligned}
\operatorname{span}\{\tilde{\mathbf{v}}_{-1}, \tilde{\mathbf{v}}_0, \ldots, \tilde{\mathbf{v}}_{-k}, \tilde{\mathbf{v}}_{k-1}\} &= \operatorname{span}\{\tilde{\mathbf{v}}_{-1}, \tilde{\mathbf{v}}_0, \ldots, \tilde{\mathbf{v}}_{-k}, U^{k-1}\mathbf{h}\} \\
&= \operatorname{span}\{\tilde{\mathbf{v}}_{-1}, \tilde{\mathbf{v}}_0, \ldots, \tilde{\mathbf{v}}_{-k}, \mathbf{w}_{k-1}\},
\end{aligned}$$

where the second equality is justified by the observation made in the previous paragraph, inducing equality (13). Equality (14) can be deduced using the same reasoning as for Eq. (13) by interchanging the roles of $(\tilde{\mathbf{v}}_k)$ and $(\mathbf{w}_k)$. □

Equalities (12)–(14) are due to the crosses linking the sequences corresponding to $(\tilde{\mathbf{v}}_k)$ and $(\mathbf{w}_k)$, whereas equalities (15)–(17) are due to the crosses linking the sequences corresponding to $(\mathbf{w}_k)$ and $(\mathbf{v}_k)$. The columns in Fig. 6 determine the order in which the orthonormal vectors will be computed. Intuitively each cross in Fig. 6 represents a coupled two term recurrence. Going through the pattern of crosses, the orthonormal vectors are computed columnwise. Note that $(\tilde{\mathbf{v}}_k)$ is only utilized to connect $(\mathbf{v}_k)$ and $(\mathbf{w}_k)$, and does not appear explicitly in the recurrences.

As an example for the application of Lemma 3, consider the computation of $\mathbf{v}_2$, $\tilde{\mathbf{v}}_1$ and $\mathbf{w}_{-2}$, i.e., the fourth column of orthonormal vectors to be computed in Fig. 6. To compute $\mathbf{w}_{-2}$ one has to orthonormalize $U^{-2}\mathbf{h}$ against $\mathbf{w}_0$, $\mathbf{w}_{-1}$ and $\mathbf{w}_1$. Equation (14) implies that $U^{-2}\mathbf{h}$ can by replaced by $\tilde{\mathbf{v}}_{-2}$ without altering the resulting vector $\mathbf{w}_{-2}$, i.e., one can orthonormalize $\tilde{\mathbf{v}}_{-2}$ against $\mathbf{w}_0$, $\mathbf{w}_{-1}$ and $\mathbf{w}_1$ in order to obtain $\mathbf{w}_{-2}$. As $\tilde{\mathbf{v}}_{-2}$ is already orthogonal to

$$\operatorname{span}\{\mathbf{w}_0, \mathbf{w}_{-1}\} = \operatorname{span}\{\mathbf{h}, U^{-1}\mathbf{h}\} = \operatorname{span}\{\tilde{\mathbf{v}}_{-1}, \tilde{\mathbf{v}}_0\},$$

where the latter is due to (12), $\mathbf{w}_{-2}$ is the result of orthonormalizing $\tilde{\mathbf{v}}_{-2}$ against $\mathbf{w}_1$. Analogously, $\tilde{\mathbf{v}}_1$ which is part of the same cross structure as $\mathbf{w}_{-2}$ is the result of orthonormalizing $\mathbf{w}_1$ against $\tilde{\mathbf{v}}_{-2}$. The vector $\mathbf{v}_2$ is computed as $U\tilde{\mathbf{v}}_1$.

In general, by the same reasoning as in the previous paragraph, the crosses connecting the sequences corresponding to $(\tilde{\mathbf{v}}_k)$ and $(\mathbf{w}_k)$ give rise to the recurrence relations

$$\begin{aligned}\tilde{\mathbf{v}}_k\beta_k &= \mathbf{w}_k + \tilde{\mathbf{v}}_{-k-1}\alpha_k,\\ \mathbf{w}_{-k-1}\beta_k &= \tilde{\mathbf{v}}_{-k-1} + \mathbf{w}_k\bar{\alpha}_k,\end{aligned}$$

or equivalently

$$\begin{aligned}\mathbf{v}_{k+1}\beta_k &= U\mathbf{w}_k + \mathbf{v}_{-k}\alpha_k,\\ \mathbf{w}_{-k-1}\beta_k &= U^{-1}\mathbf{v}_{-k} + \mathbf{w}_k\bar{\alpha}_k,\end{aligned}$$

where

$$\alpha_k = -\langle U\mathbf{w}_k, \mathbf{v}_{-k}\rangle, \qquad \beta_k = \sqrt{1 - |\alpha_k|^2}.$$

The crosses linking the sequences corresponding to $(\mathbf{v}_k)$ and $(\mathbf{w}_k)$ give rise to the recurrence relations

$$\begin{aligned}\mathbf{w}_{k+1}\epsilon_k &= \mathbf{v}_{k+1} + \mathbf{w}_{-k-1}\delta_k,\\ \mathbf{v}_{-k-1}\epsilon_k &= \mathbf{w}_{-k-1} + \mathbf{v}_{k+1}\bar{\delta}_k,\end{aligned}$$

where

$$\delta_k = -\langle \mathbf{v}_{k+1}, \mathbf{w}_{-k-1}\rangle, \qquad \epsilon_k = \sqrt{1 - |\delta_k|^2}.$$

Consequently, we have rediscovered the recurrence relations discussed in [15] for computing the bases $(\mathbf{v}_k)$ and $(\mathbf{w}_k)$ simultaneously. Given the recurrence relations, one can see that the matrix of U with respect to the bases $(\mathbf{w}_k)$ and $(\mathbf{v}_k)$ is given by the matrix

$$X = \mathbf{V}^* U \mathbf{W} = \begin{bmatrix} -\alpha_0 & \beta_0 & & & & & \\ \beta_0 & \bar{\alpha}_0 & & & & & \\ & & -\alpha_1 & \beta_1 & & & \\ & & \beta_1 & \bar{\alpha}_1 & & & \\ & & & & -\alpha_2 & \beta_2 & \\ & & & & \beta_2 & \bar{\alpha}_2 & \\ & & & & & & \ddots \end{bmatrix},$$

and the matrix of the identity operator with respect to the bases $(\mathbf{v}_k)$ and $(\mathbf{w}_k)$ is given by the matrix

$$Y = \mathbf{W}^* I \mathbf{V} = \begin{bmatrix} 1 & & & & & & & \\ & -\delta_0 & \varepsilon_0 & & & & & \\ & \varepsilon_0 & \bar{\delta}_0 & & & & & \\ & & & -\delta_1 & \varepsilon_1 & & & \\ & & & \varepsilon_1 & \bar{\delta}_1 & & & \\ & & & & & -\delta_2 & \varepsilon_2 & \\ & & & & & \varepsilon_2 & \bar{\delta}_2 & \\ & & & & & & & \ddots \end{bmatrix}.$$

Hence, the matrix of U with respect to the bases $(\mathbf{v}_k)$ is given by XY, which is a matrix of pentadiagonal form, as already shown in Sect. 3.2.

4.2 The swapping procedure

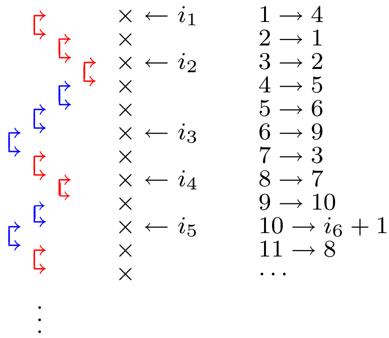
In this section the technique of swapping elements as described in Subsect. 4.1 will be generalized, with the intention of determing two term recurrences for arbitrary extended Krylov sequences for unitary matrices.

We will explain this by means of an example. Consider the pattern of rotations as depicted in Fig. 7, which corresponds to the sequence

$$\mathbf{h},\ U\mathbf{h},\ U^2\mathbf{h},\ U^{-1}\mathbf{h},\ U^{-2}\mathbf{h},\ U^{-3}\mathbf{h},\ U^3\mathbf{h},\ U^4\mathbf{h},\ U^{-4}\mathbf{h},\ U^{-5}\mathbf{h},\ U^5\mathbf{h},\ \ldots. \tag{18}$$

The pattern of rotations as depicted in Fig. 7 consists of four columns. From the sequence (18) four additional sequences will be constructed, denoted with auxiliary sequence 1 up to 4. These sequences are depicted in Fig. 8. The first auxiliary sequence is obtained by multiplying sequence (18) with U^{-1}. Next we apply to the first auxiliary sequence what we will call the *swapping procedure*. The second auxiliary sequence is obtained by swapping neighbouring elements in the first auxiliary sequence whenever there is a rotation acting on the same positions in the first column of the pattern

Fig. 7 Graphical representation of the swapping procedure



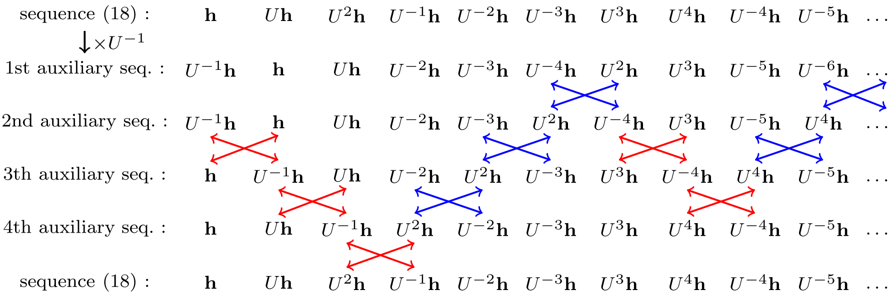


Fig. 8 The swapping procedure applied

of rotations (7). The third auxiliary sequence is obtained by swapping neighbouring elements in the second auxiliary sequence whenever there is a rotation acting on the same positions in the second column of the pattern of rotations (7) and finally the fourth auxiliary sequence is obtained by swapping neighbouring elements in the third sequence whenever there is a rotation acting on the same positions in the third column of the pattern of rotations (7). The essence of the method is that by swapping neighbouring elements in the fourth (final) auxiliary sequence whenever there is a rotation acting on the same positions in the fourth (last) column of the pattern of rotations, one obtaines the original sequence (18). In order to prove this, consider Fig. 7 where the result of the swapping procedure is shown, i.e., when applied to some sequence of vectors, the vector in the first position is transfered to the fourth position, the vector in the second position is transfered to the first position, and so on. Note that the pattern of rotations can be divided into two subsequences, a sequence corresponding to ascending exponents which is highlighted in red and a sequence corresponding to descending exponents which is highlighted in blue. As is depicted in Fig. 7, if the ith rotation is highlighted in red, the ith element of the sequence is mapped to the jth element, where the jth rotation is the last rotation highlighted in red and preceding the ith one. If the ith rotation is highlighted in blue, the ith element of the sequence is mapped to the jth element, where the jth rotation is the first rotation highlighted in blue and following the ith one. In other words, applying the swapping procedure is indentical with multiplication by U. Therefore, applying the swapping

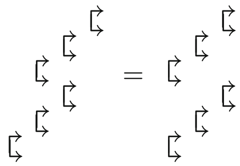


Fig. 9 Two patterns of rotations representing the same unitary matrix

procedure to the first auxiliary sequence, the latter being the original sequence (18) times U^{-1}, returns the original sequence (18).

Obviously, the same reasoning applies to any patterns of rotations and the associated number of sequences to be generated.

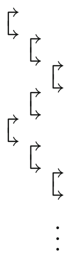
Remark 2 In order to compute an extended Krylov basis, the algorithm presented below introduces additional bases which are coupled with the latter basis and with each other by two term recurrences. These additional bases are created by the swapping procedure as described in this section. The number of additional bases is determined by the number of columns of the corresponding pattern of rotations. Sometimes the number of additional bases can be reduced by rewriting the pattern of rotations. Consider Fig. 9. On the left a rotation pattern is shown consisting of four columns, whereas on the right a pattern of rotations is depicted consisting of only three columns, though both patterns represent the same matrix. Therefore, applying the algorithm described below on the left pattern will give rise to the computation of four additional bases and a factorization of the corresponding extended Hessenberg matrix comprised of four factor matrices, whereas applying the same algorithm on the left pattern will give rise to the computation of three additional bases and a factorization of the same extended Hessenberg matrix comprised of three factor matrices.

4.3 Two periodic pattern of rotations

Our aim is to apply the swapping procedure of Sect. 4.2 to arbitrary extended Krylov sequences. As an example to describe our method, we orthonormalize the sequence

$$\mathbf{h}, U\mathbf{h}, U^2\mathbf{h}, U^{-1}\mathbf{h}, U^{-2}\mathbf{h}, U^3\mathbf{h}, U^4\mathbf{h}, U^{-3}\mathbf{h}, U^{-4}\mathbf{h}, \ldots,$$

of which the position vector corresponds to the pattern of rotations (19).



(19)

The pattern (19) consists of three columns, hence we will simultaneously orthonormalize four sequences giving rise to the bases $(\mathbf{v}_k)$, $(\tilde{\mathbf{v}}_k)$, $(\mathbf{w}_k)$ and $(\mathbf{u}_k)$. First

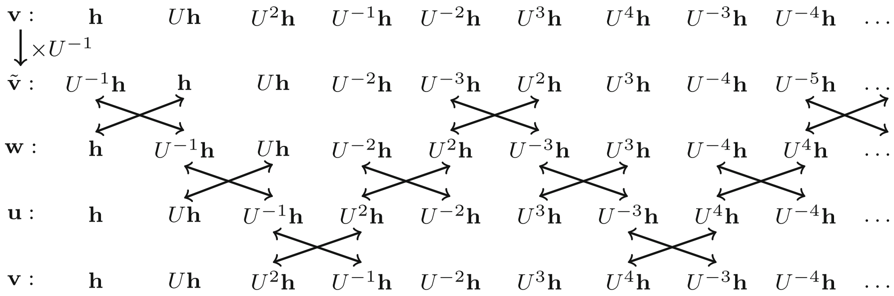


Fig. 10 Links between the sequences corresponding to the bases (v_k), (w_k) and (u_k)

the sequence corresponding to $(\tilde{\mathbf{v}}_k)$ is constructed by multiplying the vectors of the sequence corresponding to $(\mathbf{v}_k)$ with U^{-1}. The sequence corresponding to $(\mathbf{w}_k)$ can be derived from that of $(\tilde{\mathbf{v}}_k)$ by swapping neighbouring elements whenever there is a rotation acting on the same positions in the first column. The sequence corresponding to $(\mathbf{u}_k)$ can be derived from that of $(\mathbf{w}_k)$ by swapping neighbouring elements whenever there is a rotation acting on the same positions in the second column. And finally, the sequence corresponding to $(\mathbf{v}_k)$ can be derived from that of $(\mathbf{u}_k)$ be swapping neighbouring elements whenever there is a rotation acting on the same positions in the third column. This links all three sequences in a cyclic way and is depicted in Fig. 10. Note that the arrows in Fig. 10 follow the same pattern as the rotations in (19), i.e., if we go the left in the pattern of rotations (19), we go down in Fig. 10; if we go the right in the pattern of rotations (19), we go up in Fig. 10.

Using Fig. 10, similar equalities between the spans of several subspaces can be deduced as in Lemma 3. Again the crosses connecting the different vectors contain all necessary information. Suppose we have an orthonormal vector $\mathbf{y}$ of which the underlying product of a power of U with $\mathbf{h}$ is located in the right column of a cross. Then the span of all vectors in the corresponding basis computed before $\mathbf{y}$, including $\mathbf{y}$ itself, remains the same if $\mathbf{y}$ is replaced by the orthonormal vector which is connected to $\mathbf{y}$ by the cross. We do not write down these equalities since it would make our discussion unnecessarily complicated (due to the heavy use of indices) and would not contribute to the insight Fig. 10 already provides us. Instead, we rely on Fig. 11, which gives a schematic view on the order of computation of the orthonormal vectors.

Figure 11 should be read together with Fig. 10. The orthonormal vectors are computed column by column. In each column, vectors which are located in a black disk are orthonormalized first. Vectors in the same column which are connected to each other with a solid line result in the same orthonormal vector. The dashed line represents the relation $\tilde{\mathbf{v}}_k = U^{-1}\mathbf{v}_{k+1}$.

To illustrate this, suppose we want to compute the fifth column in Fig. 10, i.e., the orthonormal vectors $\mathbf{v}_{-2}$, $\tilde{\mathbf{v}}_{-3}$, $\mathbf{w}_2$ and $\mathbf{u}_{-2}$. The vectors $\mathbf{w}_2$ and $\mathbf{u}_{-2}$ are marked with a black circle in Fig. 11 and are calculated first. The vector $\mathbf{w}_2$ is the result of orthonormalizing $U^2\mathbf{h}$ against $\mathbf{w}_0$, $\mathbf{w}_{-1}$, $\mathbf{w}_1$ and $\mathbf{w}_{-2}$. As $\mathbf{u}_2$ is a linear combination of $\mathbf{h}$, $U\mathbf{h}$, $U^{-1}\mathbf{h}$ and $U^2\mathbf{h}$ with a nonzero component in the direction of $U^2\mathbf{h}$, $U^2\mathbf{h}$ can be replaced by $\mathbf{u}_2$ without altering the resulting vector $\mathbf{w}_2$, i.e., the vector $\mathbf{w}_2$ is the result of orthonormalizing $\mathbf{u}_2$ against $\mathbf{w}_0$, $\mathbf{w}_{-1}$, $\mathbf{w}_1$ and $\mathbf{w}_{-2}$. Since $\mathbf{u}_2$ is already orthogonal to

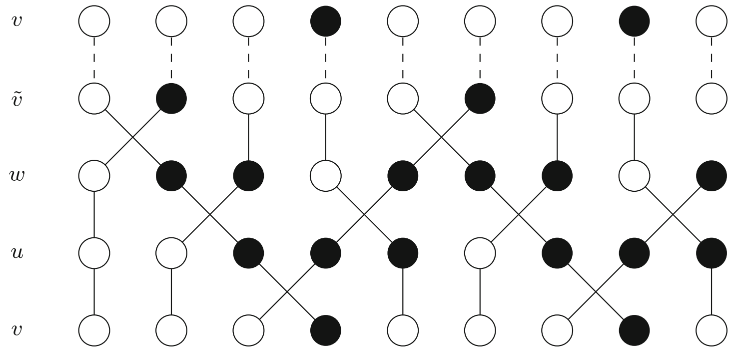


Fig. 11 Schematic view on the order of computation of the orthonormal vectors

$$\mathrm{span}\{\mathbf{u}_0, \mathbf{u}_1, \mathbf{u}_{-1}\} = \mathrm{span}\{\mathbf{h}, U\mathbf{h}, U^{-1}\mathbf{h}\} = \mathrm{span}\{\mathbf{w}_0, \mathbf{w}_{-1}, \mathbf{w}_1\},$$

$\mathbf{w}_2$ is the result of orthonormalizing $\mathbf{u}_2$ against $\mathbf{w}_{-2}$. Similarly, $\mathbf{u}_{-2}$ is the result of orthonormalizing $\mathbf{w}_{-2}$ against $\mathbf{u}_2$. One obtains the recurrence relations

$$\begin{aligned} \mathbf{w}_2\varepsilon_1 &= \mathbf{u}_2 + \mathbf{w}_{-2}\delta_1, \\ \mathbf{u}_{-2}\varepsilon_1 &= \mathbf{w}_{-2} + \mathbf{u}_2\bar{\delta}_1, \end{aligned}$$

where

$$\delta_1 = -\langle \mathbf{u}_2, \mathbf{w}_{-2} \rangle, \qquad \varepsilon_1 = \sqrt{1 - |\delta_1|^2}.$$

The vector $\mathbf{v}_{-2}$ is marked with a white circle and connected by a solid line with $\mathbf{u}_{-2}$. At the same time it is connected by a dashed line with $\tilde{\mathbf{v}}_{-3}$. The vector $\mathbf{v}_{-2}$ is the result of orthonormalizing $U^{-2}\mathbf{h}$ against

$$\mathrm{span}\{\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_{-1}\} = \mathrm{span}\{\mathbf{h}, U\mathbf{h}, U^2\mathbf{h}, U^{-1}\mathbf{h}\},$$

whereas the vector $\mathbf{u}_{-2}$ is the result of orthonormalizing $U^{-2}\mathbf{h}$ against

$$\mathrm{span}\{\mathbf{u}_0, \mathbf{u}_1, \mathbf{u}_{-1}, \mathbf{u}_2\} = \mathrm{span}\{\mathbf{h}, U\mathbf{h}, U^{-1}\mathbf{h}, U^2\mathbf{h}\}.$$

The latter implies that $\mathbf{v}_{-2}$ and $\mathbf{u}_{-2}$ are obtained by orthonormalizing $U^{-2}\mathbf{h}$ against the same subspace, implying that both vectors are equal up to a unimodular factor, which we choose to be one. Therefore, one obtains

$$\mathbf{v}_{-2} = \mathbf{u}_{-2}.$$

Finally, by construction one has

$$\tilde{\mathbf{v}}_{-3} = U^{-1}\mathbf{v}_{-2}.$$

In this way one proceeds columnwise, computing the bases $(\mathbf{v}_k)$, $(\mathbf{w}_k)$ and $(\mathbf{u}_k)$ simultaneously.

The matrix of U with respect to the bases $(\mathbf{w}_k)$ and $(\mathbf{v}_k)$ is given by the matrix

$$X = \mathbf{V}^* U \mathbf{W} = \begin{bmatrix} -\alpha_0 & \beta_0 & & & & & & \\ \beta_0 & \bar{\alpha}_0 & & & & & & \\ & & 1 & & & & & \\ & & & 1 & & & & \\ & & & & -\alpha_1 & \beta_1 & & \\ & & & & \beta_1 & \bar{\alpha}_1 & & \\ & & & & & & 1 & \\ & & & & & & & \ddots \end{bmatrix},$$

the matrix of the identity operator with respect to the bases $(\mathbf{u}_k)$ and $(\mathbf{w}_k)$ is given by the matrix

$$Y = \mathbf{W}^* I \mathbf{U} = \begin{bmatrix} 1 & & & & & & & \\ & -\delta_0 & \varepsilon_0 & & & & & \\ & \varepsilon_0 & \bar{\delta}_0 & & & & & \\ & & & -\delta_1 & \varepsilon_1 & & & \\ & & & \varepsilon_1 & \bar{\delta}_1 & & & \\ & & & & & -\delta_2 & \varepsilon_2 & \\ & & & & & \varepsilon_2 & \bar{\delta}_2 & \\ & & & & & & & \ddots \end{bmatrix},$$

and the matrix of the identity operator with respect to the bases $(\mathbf{v}_k)$ and $(\mathbf{u}_k)$ is given by the matrix

$$Z = \mathbf{U}^* I \mathbf{V} = \begin{bmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & -\xi_0 & \gamma_0 & & & \\ & & \gamma_0 & \bar{\xi}_0 & & & \\ & & & & 1 & & \\ & & & & & 1 & \\ & & & & & & \ddots \end{bmatrix}.$$

The product XYZ is an extended Hessenberg matrix corresponding to the position vector $\mathbf{p} = [\ell, \ell, r, r, \ell, \ell, \ldots]$.

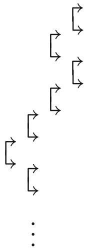
4.4 Arbitrary rotation patterns and algorithm

In this section a new algorithm is presented for computing an orthonormal extended Krylov basis. Algorithm 2 returns an orthonormal basis $(\mathbf{v}_k)$ for an arbitrary extended Krylov subspace, given a unitary matrix U, a starting vector $\mathbf{h}$ and a position vector

p determining the ordering of the extended Krylov sequence. Together with the basis vectors $(\mathbf{v}_k)$ the corresponding extended Hessenberg matrix H, i.e., the projection of U on the extended Krylov subspace, is returned. When examining Algorithm 2, note that to compute the upper left $m \times m$ submatrix of H correctly, a position vector of length m is required. We will now explain the mechanics of the algorithm by means of an example. Consider the extended Krylov sequence

$$\mathbf{h},\ U^{-1}\mathbf{h},\ U\mathbf{h},\ U^{-2}\mathbf{h},\ U^{-3}\mathbf{h},\ U^{-4}\mathbf{h},\ U^{2}\mathbf{h},\ \ldots,$$

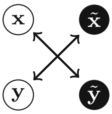
corresponding to the position vector $\mathbf{p} = [r, \ell, r, r, r, \ell, \ldots]$ and therefore to the pattern of rotations (20).



(20)

The pattern (20) consists of four columns, hence in addition to the sequences $(\mathbf{w}_k)$ and $(\mathbf{u}_k)$ an extra sequence $(\mathbf{z}_k)$ is needed. This is visualized in Fig. 12.

Figure 13 shows the order in which the orthonormal vectors are computed. Given this and the examples of the previous subsections, the building blocks for a general algorithm can be constructed. Vectors which are part of a cross structure in Figs. 12 and 13 are computed by the recurrence relations



$$\tilde{\mathbf{x}}\beta = \mathbf{y} + \mathbf{x}\alpha,$$

$$\tilde{\mathbf{y}}\beta = \mathbf{x} + \mathbf{y}\bar{\alpha},$$

$$\begin{array}{llcccccccc}
 & \mathbf{v}: & \mathbf{h} & U^{-1}\mathbf{h} & U\mathbf{h} & U^{-2}\mathbf{h} & U^{-3}\mathbf{h} & U^{-4}\mathbf{h} & U^{2}\mathbf{h} & \ldots \\
 & \downarrow \times U^{-1} & & & & & & & & \\
row\,1 \rightarrow & \tilde{\mathbf{v}}: & U^{-1}\mathbf{h} & U^{-2}\mathbf{h} & \mathbf{h} & U^{-3}\mathbf{h} & U^{-4}\mathbf{h} & U^{-5}\mathbf{h} & U\mathbf{h} & \ldots \\
row\,2 \rightarrow & \mathbf{w}: & U^{-1}\mathbf{h} & U^{-2}\mathbf{h} & \mathbf{h} & U^{-3}\mathbf{h} & U^{-4}\mathbf{h} & U\mathbf{h} & U^{-5}\mathbf{h} & \ldots \\
row\,3 \rightarrow & \mathbf{u}: & U^{-1}\mathbf{h} & U^{-2}\mathbf{h} & \mathbf{h} & U^{-3}\mathbf{h} & U\mathbf{h} & U^{-4}\mathbf{h} & U^{2}\mathbf{h} & \ldots \\
row\,4 \rightarrow & \mathbf{z}: & U^{-1}\mathbf{h} & \mathbf{h} & U^{-2}\mathbf{h} & U\mathbf{h} & U^{-3}\mathbf{h} & U^{-4}\mathbf{h} & U^{2}\mathbf{h} & \ldots \\
 & \mathbf{v}: & \mathbf{h} & U^{-1}\mathbf{h} & U\mathbf{h} & U^{-2}\mathbf{h} & U^{-3}\mathbf{h} & U^{-4}\mathbf{h} & U^{2}\mathbf{h} & \ldots
\end{array}$$

Fig. 12 Links between the sequences corresponding to $(\mathbf{v}_k)$, $(\mathbf{w}_k)$, $(\mathbf{u}_k)$ and $(\mathbf{z}_k)$

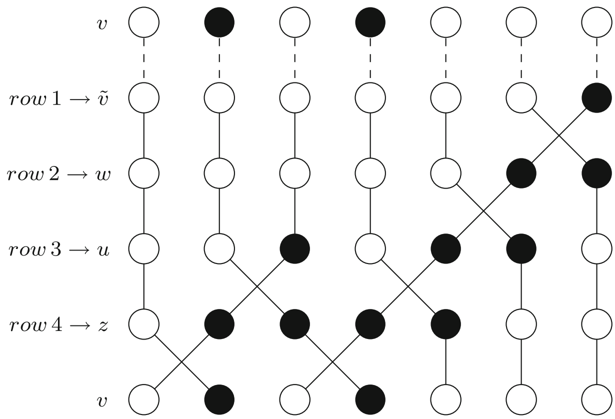


Fig. 13 Schematic view on the order of computation of the orthonormal vectors

where $\alpha = -\langle \mathbf{y}, \mathbf{x} \rangle$ and $\beta = \sqrt{1 - |\alpha|^2}$. The coefficients α and β are stored as they are part of the sparse factorization of the corresponding extended Hessenberg matrix.

Orthonormal vectors which are connected with a solid line in Fig. 13 are the same. The dashed line indicates multiplication with U, i.e., for each $k \in \mathbb{Z}$, $\mathbf{v}_k = U\tilde{\mathbf{v}}_{k-1}$. As the vectors indicated with a black disk are computed first, the vectors indicated with a white disk are found at once. This allows us to run through Fig. 13 column by column, computing the bases $(\mathbf{v}_k)$, $(\mathbf{w}_k)$, $(\mathbf{u}_k)$ and $(\mathbf{z}_k)$ simultaneously. Note that as our main interest is to compute the basis $(\mathbf{v}_k)$, we do not need to store the whole bases $(\tilde{\mathbf{v}}_k)$, $(\mathbf{w}_k)$, $(\mathbf{u}_k)$ and $(\mathbf{z}_k)$, but only the most recently computed vectors of the latter bases as these are the vectors necessary to compute the next basis vector of $(\mathbf{v}_k)$.

We will now clarify some of the notation used in Algorithm 2. In contrast to the rest of the manuscript, the orthonormal basis vectors $(\mathbf{v}_k)$ are indexed linearly, i.e., k denotes the order in which the vectors are computed, starting with $\mathbf{v}_1$. In each iteration only the most recently computed vectors of the auxiliary bases need to be stored, these are denoted by the vectors $\mathbf{w}_1, \ldots, \mathbf{w}_{width}$. In the example above $width = 4$ and $\mathbf{w}_1$, $\mathbf{w}_2$, $\mathbf{w}_3$, $\mathbf{w}_4$ correspond to the most recently computed vector of the bases $(\tilde{\mathbf{v}}_k)$, $(\mathbf{w}_k)$, $(\mathbf{u}_k)$ and $(\mathbf{z}_k)$ respectively. Note that the variable $width$ corresponds with the width of the pattern (20). Finally, the vector row is used to keep track of the current location in the pattern. More specifically, $row(i)$ indicates the row number of the upper left element of the ith cross. In the example of Fig. 13 we have $row = [4, 3, 4, 3, 2, 1, \ldots]$. The vector row is easily obtained from the position vector $\mathbf{p}$.

Algorithm 2 clearly exhibits a computational advantage with respect to the classical Arnoldi algorithm, as in each iteration only one inner product needs to be computed. In order to gain this computational advantage, w extra bases need to be computed simultaneously with the original extended Krylov basis, where w is the width of the corresponding pattern of rotations. The width w of this pattern is at most equal to the number of orthonormal vectors to be retrieved, i.e., when the position vector $\mathbf{p}$ consists entirely of ℓ's or entirely of r's. As we only need to store the most recently computed orthonormal vectors of this extra bases, the memory cost of Algorithm 2 is at worst twice as high as the memory cost of Arnoldi. Another advantage of Algorithm 2 is

Algorithm 2 Algorithm for computing orthonormal extended Krylov bases for unitary matrices.

Require: unitary matrix U, starting vector $\mathbf{h}$, position vector $\mathbf{p}$

▷ Initialization

$\mathbf{v}_1 \leftarrow \mathbf{h}/||\mathbf{h}||_2$;
for $i = 1 \rightarrow row(1)$ **do**
  $\mathbf{w}_i \leftarrow U^*\mathbf{v}_1$;
end for
for $i = row(1) + 1 \rightarrow width$ **do**
  $\mathbf{w}_i \leftarrow \mathbf{v}_1$;
end for
for $i = 1 \rightarrow width$ **do**
  $H_i = I_{length\,\mathbf{p}+1}$
end for

▷ Update vectors located in black disks

for $k = 2 \rightarrow length\,\mathbf{p} + 1$ **do**
  if $row(k-1) = width$ **then**
    $\mathbf{x} \leftarrow \mathbf{w}_{row(k-1)}$;
    $\mathbf{y} \leftarrow \mathbf{v}_{k-1}$;
    $\alpha \leftarrow -\langle \mathbf{y}, \mathbf{x} \rangle$;
    $\beta \leftarrow \sqrt{1 - \alpha\bar{\alpha}}$;
    $\mathbf{w}_{row(k-1)} \leftarrow (y + \alpha x)/\beta$;
    $\mathbf{v}_k \leftarrow (x + \bar{\alpha} y)/\beta$;
  else
    $\mathbf{x} \leftarrow \mathbf{w}_{row(k-1)}$;
    $\mathbf{y} \leftarrow \mathbf{w}_{row(k-1)+1}$;
    $\alpha \leftarrow -\langle \mathbf{y}, \mathbf{x} \rangle$;
    $\beta \leftarrow \sqrt{1 - \alpha\bar{\alpha}}$;
    $\mathbf{w}_{row(k-1)} \leftarrow (\mathbf{y} + \alpha \mathbf{x})/\beta$;
    $\mathbf{w}_{row(k-1)+1} \leftarrow (\mathbf{x} + \bar{\alpha} \mathbf{y})/\beta$;
  end if

▷ Update vectors located in white disks

  if $row(k) > row(k-1)$ **then**
    for $i = 1 \rightarrow row(k-1) - 1$ **do**
      $\mathbf{w}_i \leftarrow \mathbf{w}_{row(k-1)}$;
    end for
    $\mathbf{v}_k \leftarrow U\mathbf{w}_1$;
    for $i = row(k-1) + 2 \rightarrow width$ **do**
      $\mathbf{w}_i = \mathbf{v}_k$;
    end for
  else
    if $row(k-1) \neq width$ **then**
      for $i = row(k-1) + 2 \rightarrow width$ **do**
        $\mathbf{w}_i \leftarrow \mathbf{w}_{row(k-1)+1}$;
      end for
      $\mathbf{v}_k \leftarrow \mathbf{w}_{width}$;
      for $i = 1 \rightarrow row(k-1) - 1$ **do**
        $\mathbf{w}_i \leftarrow U^* v_k$;
      end for
    end if
  end if

▷ Update Hessenberg factorization

$$\begin{pmatrix} \left(H_{row(k-1)}\right)_{k-1,k-1} & \left(H_{row(k-1)}\right)_{k-1,k} \\ \left(H_{row(k-1)}\right)_{k,k-1} & \left(H_{row(k-1)}\right)_{k,k} \end{pmatrix} \leftarrow \begin{pmatrix} -\alpha & \beta \\ \beta & \bar{\alpha} \end{pmatrix}$$

end for
$H \leftarrow H_1 H_2 \ldots H_{width}$
return $(\mathbf{v}_k)$, H

the computation of the associated extended Hessenberg matrix H, which is returned in factored form, the factors being sparse block matrices consisting of an alternating sequence of 2×2 unitary rotations and identity blocks.

In case the position vector $\mathbf{p}$ consists of an entire sequence of ℓ's, the algorithm will compute an orthonormal Krylov basis for a unitary matrix. For this case, the reader might be interested in the isometric Arnoldi algorithm [5,6,16], which is also based on coupled two term recurrences.

5 Conclusion

We established a new proof for the general structure of the projection of a matrix onto an extended Krylov subspace, which is a matrix containing a sequence of overlapping blocks on the diagonal which are alternatingly of Hessenberg and inverse Hessenberg form. Furthermore, we characterized this matrices by means of their QR-factorization, the factor Q being a product of 2×2 unitary rotations. This allowed us to derive and extend the recurrences for Hermitian matrices as established in [7], without the use of orthonormal polynomial relations. Furthermore, we investigated the structure of unitary extended Hessenberg matrices and derived corresponding recurrences, including the CMV-form and its associated coupled two term recurrence as was established in [15].

References

1. Antoulas, A.C.: Approximation of Large-Scale Dynamical Systems. SIAM, Philadelphia (2005)
2. Barroso, R.C., Delvaux, S.: Orthogonal Laurent polynomials on the unit circle and snake-shaped matrix factorizations. J. Approx. Theory **161**(1), 65–87 (2009)
3. Cantero, M.J., Moral, L., Velazquez, L.: Five-diagonal matrices and zeros of orthogonal polynomials on the unit circle. Linear Algebra Appl. **362**, 29–56 (2003)
4. Druskin, V., Knizhnerman, L.: Extended Krylov subspaces: approximations of the matrix square root and related functions. SIAM J. Matrix Anal. Appl. **19**(3), 755–771 (1998)
5. Gragg, W.B.: The QR-algorithm for unitary Hessenberg matrices. J. Comput. Appl. Math. **16**, 1–8 (1986)
6. Gragg, W.B.: Positive definite Toeplitz matrices, the Arnoldi process for isometric operators, and Gaussian quadrature on the unit circle. J. Comput. Appl. Math. **46**(1–2), 183–198 (1993)
7. Jagels, C., Reichel, L.: The extended Krylov subspace method and orthogonal Laurent polynomials. Linear Algebra Appl. **431**(3), 441–458 (2009)
8. Knizhnerman, L., Simoncini, V.: A new investigation of the extended Krylov subspace method for matrix function evaluations. Numer. Linear Algebra Appl. **17**(4), 615–638 (2010)
9. Knizhnerman, L., Simoncini, V.: Convergence analysis of the extended Krylov subspace method for the Lyapunov equation. Numer. Math. **118**(3), 567–586 (2011)
10. Simon, B.: CMV matrices: five years after. J. Comput. Appl. Math. **208**(1), 120–154 (2007)
11. Simoncini, V.: A new iterative method for solving large scale Lyapunov matrix equations. SIAM J. Sci. Comput. **29**(3), 1268–1288 (2007)
12. Vandebril, R.: Chasing bulges or rotations? A metamorphosis of the QR-algorithm. SIAM J. Matrix Anal. Appl. **32**, 217–247 (2011)
13. Vandebril, R., Van Barel, M., Mastronardi, N.: Matrix Computations and Semiseparable Matrices, Volume I: Linear Systems. Johns Hopkins University Press, Baltimore (2008)
14. Vandebril, R., Watkins, D.S.: A generalization of the multishift QR algorithm. SIAM J. Matrix Anal. Appl. **33**(3), 759–779 (2012)
15. Watkins, D.S.: Some perspectives on the eigenvalue problem. SIAM Rev. **35**(3), 430–471 (1993)
16. Watkins, D.S.: Unitary orthogonalization processes. J. Comput. Appl. Math. **86**(1), 335–345 (1997)